

linyl, pyrazolyl, and 5,6,7,8-tetrahydroisoquinoliny. Bivalent radicals derived from univalent heteroaryl radicals whose names end in “-yl” by removal of one hydrogen atom from the atom with the free valence are named by adding “-idene” to the name of the corresponding univalent radical, e.g., a pyridyl group with two points of attachment is a pyridylidene. Heteroaryl does not encompass or overlap with aryl, cycloalkyl, or heterocycloalkyl, as defined herein

[0098] Substituted heteroaryl also includes ring systems substituted with one or more oxide (—O^-) substituents, such as pyridinyl N-oxides.

[0099] By “heterocycloalkyl” is meant a single, non-aromatic ring, usually with 3 to 7 ring atoms, containing at least 2 carbon atoms in addition to 1-3 heteroatoms independently selected from oxygen, sulfur, and nitrogen, as well as combinations comprising at least one of the foregoing heteroatoms. The ring may be saturated or have one or more carbon-carbon double bonds. Suitable heterocycloalkyl groups include, for example (as numbered from the linkage position assigned priority 1), 2-pyrrolidinyl, 2,4-imidazolidinyl, 2,3-pyrazolidinyl, 2-piperidyl, 3-piperidyl, 4-piperidyl, and 2,5-piperizinyl. Morpholinyl groups are also contemplated, including 2-morpholinyl and 3-morpholinyl (numbered wherein the oxygen is assigned priority 1). Substituted heterocycloalkyl also includes ring systems substituted with one or more oxo ($=\text{O}$) or oxide (—O^-) substituents, such as piperidinyl N-oxide, morpholinyl-N-oxide, 1-oxo-1-thiomorpholinyl and 1,1-dioxo-1-thiomorpholinyl.

[0100] “Heterocycloalkyl” also includes bicyclic ring systems wherein one non-aromatic ring, usually with 3 to 7 ring atoms, contains at least 2 carbon atoms in addition to 1-3 heteroatoms independently selected from oxygen, sulfur, and nitrogen, as well as combinations comprising at least one of the foregoing heteroatoms; and the other ring, usually with 3 to 7 ring atoms, optionally contains 1-3 heteroatoms independently selected from oxygen, sulfur, and nitrogen and is not aromatic.

[0101] As used herein, “modulation” refers to a change in activity as a direct or indirect response to the presence of compounds of Formula I, relative to the activity of in the absence of the compound. The change may be an increase in activity or a decrease in activity, and may be due to the direct interaction of the compound with the kinesin, or due to the interaction of the compound with one or more other factors that in turn affect kinesin activity. For example, the presence of the compound may, for example, increase or decrease kinesin activity by directly binding to the kinesin, by causing (directly or indirectly) another factor to increase or decrease the kinesin activity, or by (directly or indirectly) increasing or decreasing the amount of kinesin present in the cell or organism.

[0102] The term “sulfanyl” includes the groups: —S -(optionally substituted $\text{C}_1\text{—C}_6$ alkyl), —S -(optionally substituted aryl), —S -(optionally substituted heteroaryl), and —S -(optionally substituted heterocycloalkyl). Hence, sulfanyl includes the group $\text{C}_1\text{—C}_6$ alkylsulfanyl.

[0103] The term “sulfinyl” includes the groups: —S(O) -(optionally substituted $\text{C}_1\text{—C}_6$ alkyl), —S(O) -(optionally substituted aryl), —S(O) -(optionally substituted heteroaryl),

—S(O) -(optionally substituted heterocycloalkyl); and —S(O) -(optionally substituted amino).

[0104] The term “sulfonyl” includes the groups: $\text{—S(O}_2\text{)}$ -(optionally substituted $\text{C}_1\text{—C}_6$ alkyl), $\text{—S(O}_2\text{)}$ -(optionally substituted aryl), $\text{—S(O}_2\text{)}$ -(optionally substituted heteroaryl), $\text{—S(O}_2\text{)}$ -(optionally substituted heterocycloalkyl), $\text{—S(O}_2\text{)}$ -(optionally substituted alkoxy), $\text{—S(O}_2\text{)}$ -(optionally substituted aryloxy), $\text{—S(O}_2\text{)}$ -(optionally substituted heteroaryloxy), $\text{—S(O}_2\text{)}$ -(optionally substituted heterocycloxy); and $\text{—S(O}_2\text{)}$ -(optionally substituted amino).

[0105] The term “substituted”, as used herein, means that any one or more hydrogens on the designated atom or group is replaced with a selection from the indicated group, provided that the designated atom's normal valence is not exceeded. When a substituent is oxo (i.e., $=\text{O}$) then 2 hydrogens on the atom are replaced. Combinations of substituents and/or variables are permissible only if such combinations result in stable compounds or useful synthetic intermediates. A stable compound or stable structure is meant to imply a compound that is sufficiently robust to survive isolation from a reaction mixture, and subsequent formulation as an agent having at least practical utility. Unless otherwise specified, substituents are named into the core structure. For example, it is to be understood that when (cycloalkyl)alkyl is listed as a possible substituent, the point of attachment of this substituent to the core structure is in the alkyl portion.

[0106] The terms “substituted” alkyl, cycloalkyl, aryl, heterocycloalkyl, and heteroaryl, unless otherwise expressly defined, refer respectively to alkyl, cycloalkyl, aryl, heterocycloalkyl, and heteroaryl wherein one or more (such as up to 5, for example, up to 3) hydrogen atoms are replaced by a substituent independently chosen from:

[0107] —R^a , —OR^b , optionally substituted amino (including $\text{—NR}^c\text{COR}^b$, $\text{NR}^c\text{CO}_2\text{R}^a$, $\text{—NR}^c\text{CONR}^b\text{R}^c$, $\text{—NR}^b\text{C(NR}^c\text{)NR}^b\text{R}^c$, $\text{—NR}^b\text{C(NCN)NR}^b\text{R}^c$, and $\text{—NR}^c\text{SO}_2\text{R}^a$), halo, cyano, nitro, oxo (as a substituent for cycloalkyl, heterocycloalkyl, and heteroaryl), optionally substituted acyl (such as —COR^b), optionally substituted alkoxy carbonyl (such as $\text{—CO}_2\text{R}^b$), aminocarbonyl (such as $\text{—CONR}^b\text{R}^c$), —OCOR^b , $\text{—OCO}_2\text{R}^a$, $\text{—OCONR}^b\text{R}^c$, sulfanyl (such as SR^b), sulfinyl (such as —SOR^a), and sulfonyl (such as $\text{—SO}_2\text{R}^a$ and $\text{—SO}_2\text{NR}^b\text{R}^c$),

[0108] where R_a is chosen from optionally substituted $\text{C}_1\text{—C}_6$ alkyl, optionally substituted cycloalkyl, optionally substituted heterocycloalkyl, optionally substituted alkenyl, optionally substituted alkynyl, optionally substituted aryl, and optionally substituted heteroaryl;

[0109] R_b is chosen from hydrogen, optionally substituted $\text{C}_1\text{—C}_6$ alkyl, optionally substituted cycloalkyl, optionally substituted heterocycloalkyl, optionally substituted aryl, and optionally substituted heteroaryl; and

[0110] R^c is independently chosen from hydrogen and optionally substituted $\text{C}_1\text{—C}_4$ alkyl; or

[0111] R_b and R^c , and the nitrogen to which they are attached, form an optionally substituted heterocycloalkyl group; and

[0112] where each optionally substituted group is unsubstituted or independently substituted with one or more, such as one, two, or three, substituents independently selected